

n,n-bis(2-cyanoethyl)aspartic acid
6328-90-1 | DTXSID20286167

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 267 °C

Global applicability domain: Outside

Local applicability domain index: 1.37e-01

Confidence level: 7.01e-01

Nearest Neighbors from the Training Set

Image not found

Diphenylurea

Measured: 262

Predicted: 269

Image not found

N-(4-Bromophenyl)urea

Measured: 260

Predicted: 256

Image not found

1-Phenylurea

Measured: 238

Predicted: 247

Image not found

1H-Imidazole-4-carboxylic acid

Measured: 295

Predicted: 284